

How Do We Know that Aerosol Forecasts are Improving for the Right Reasons ?

Using Testbeds to Address Modeling Challenges

Jerome Fast, Pacific Northwest National Laboratory

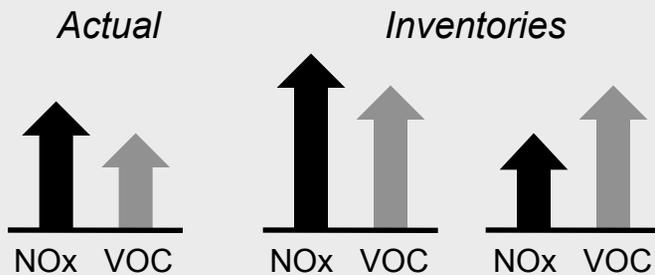
IWAQFR, Boulder CO, December 2, 2009

Air Quality Forecasts

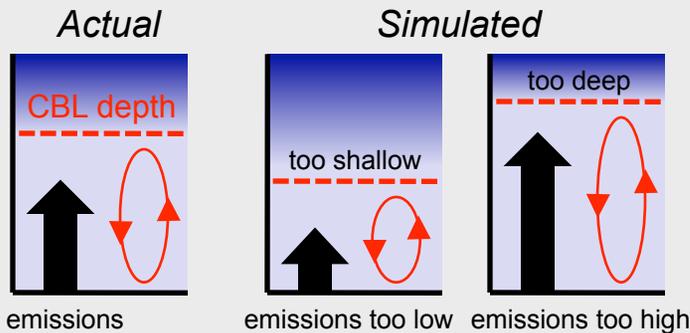
Examples of 'Getting the Right Answer for the Wrong Reasons'

Ozone Mixing Ratios

- Emission uncertainties

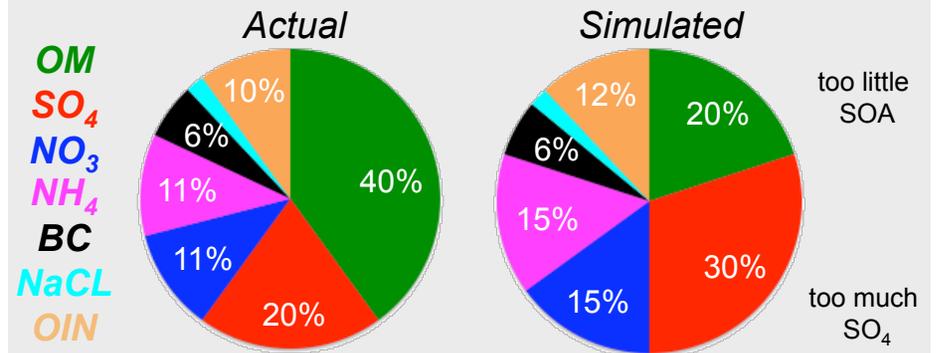


- Meteorological uncertainties

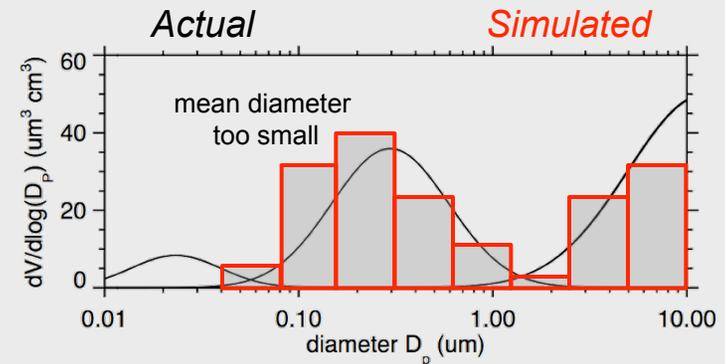


Particulate Concentrations

- Secondary formation uncertainties



- Size distribution uncertainties

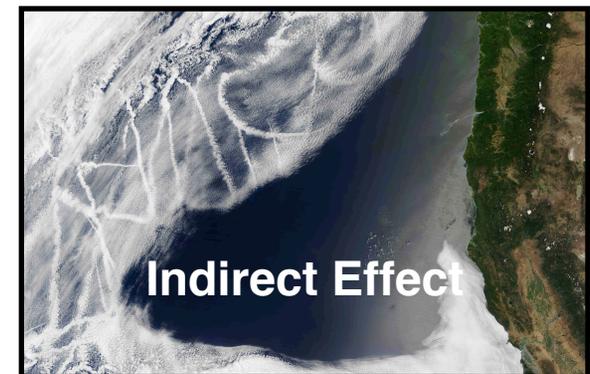
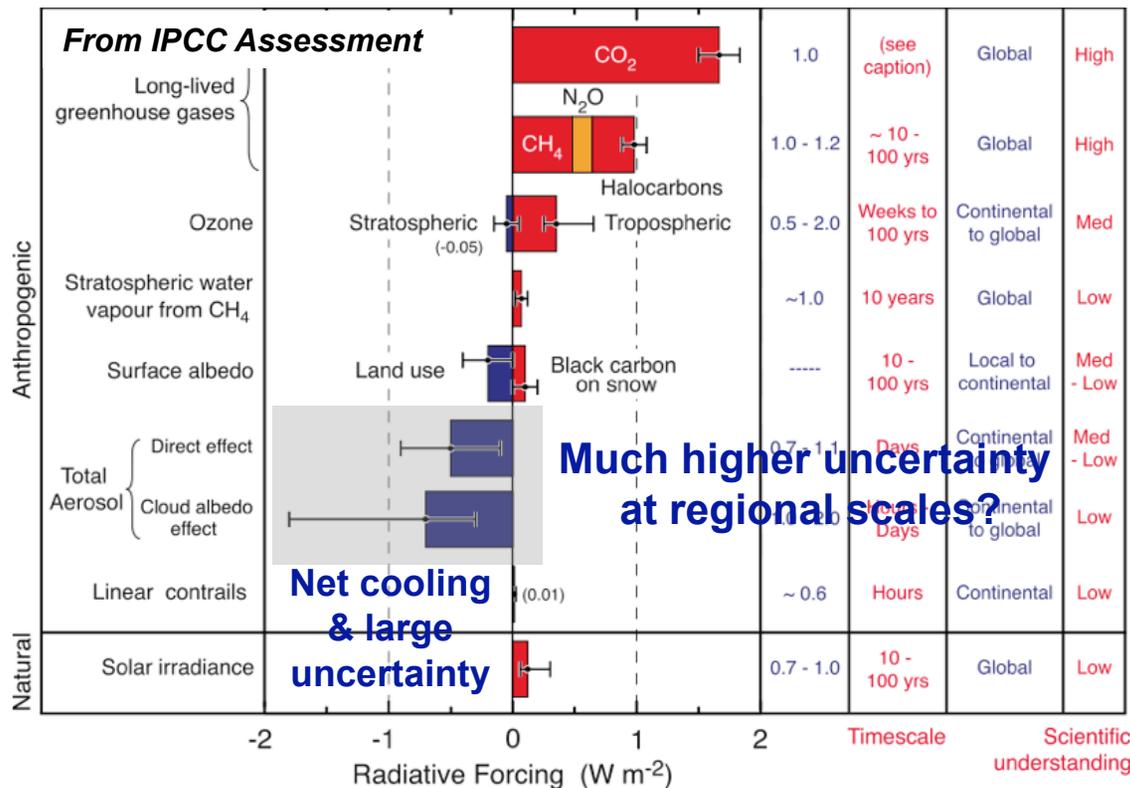


Many other more complicated relationships, compensating errors

Climate Predictions

Likewise, Radiative Forcing Can be Correct for the Wrong Reasons

- Climate models suffer from same compensative errors, although they employ simpler treatments for aerosols than air quality models
- Treatments in climate models becoming more complex as a result of more advanced computational resources



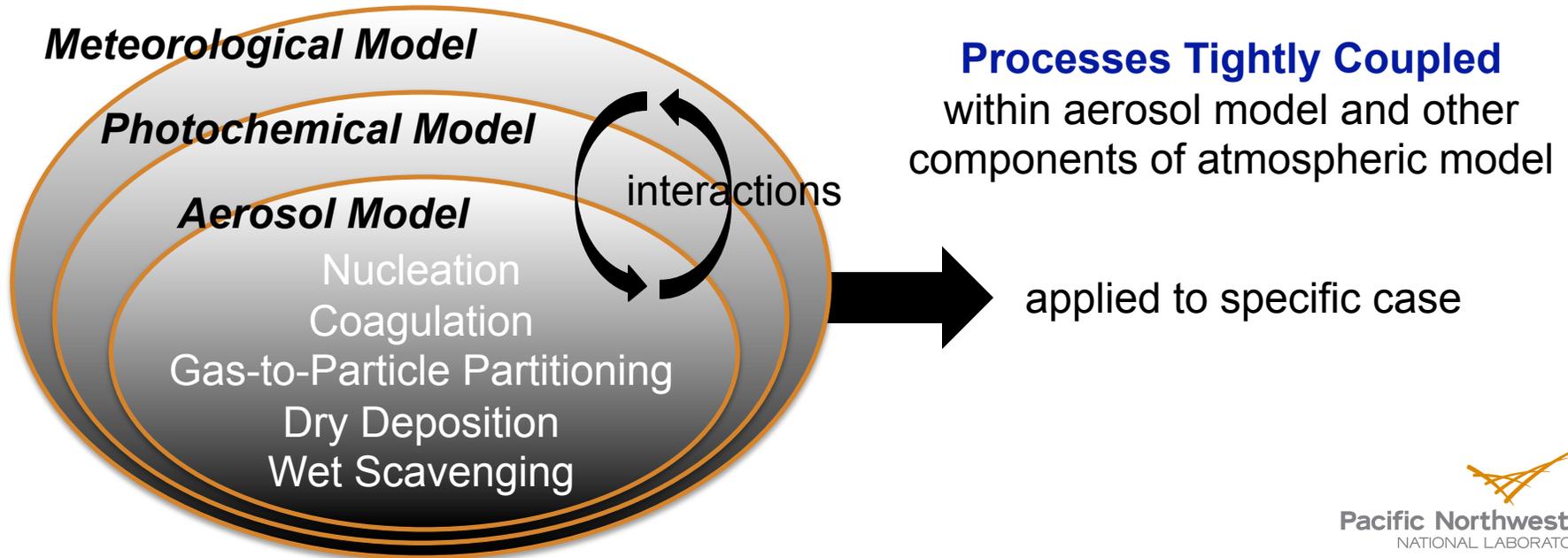
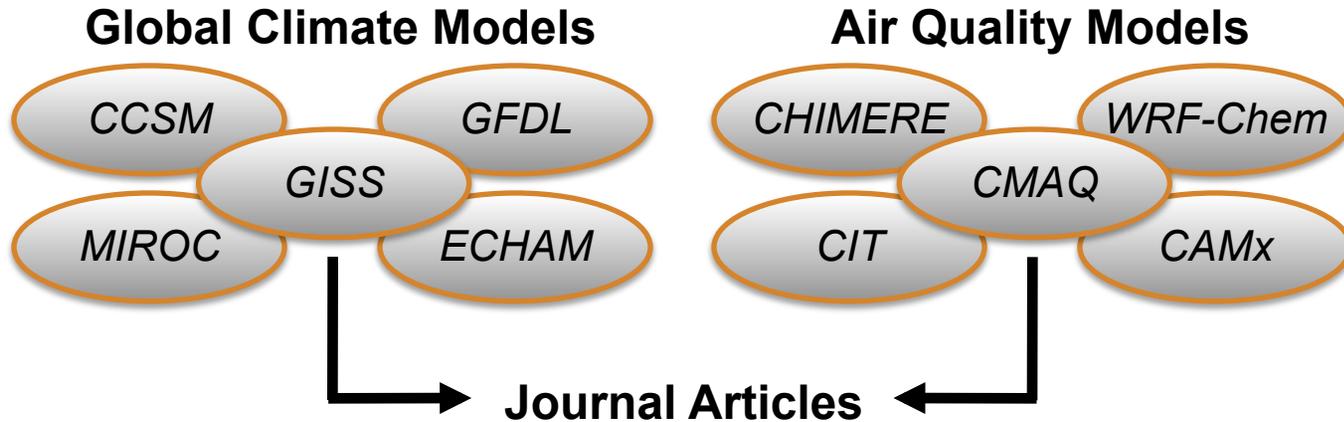
Why is there so much uncertainty ?



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Traditional Modeling Paradigm

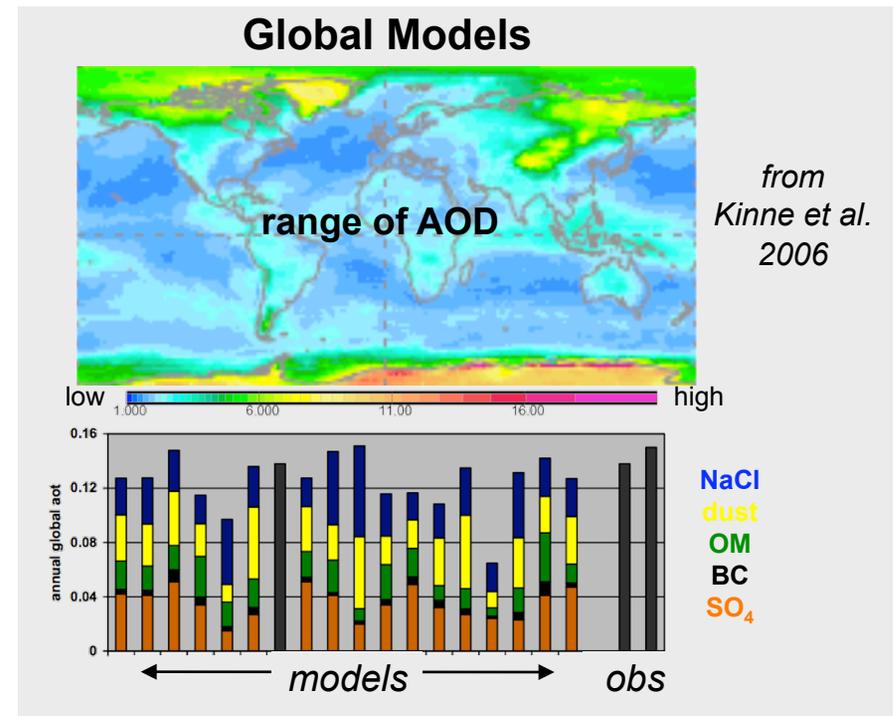
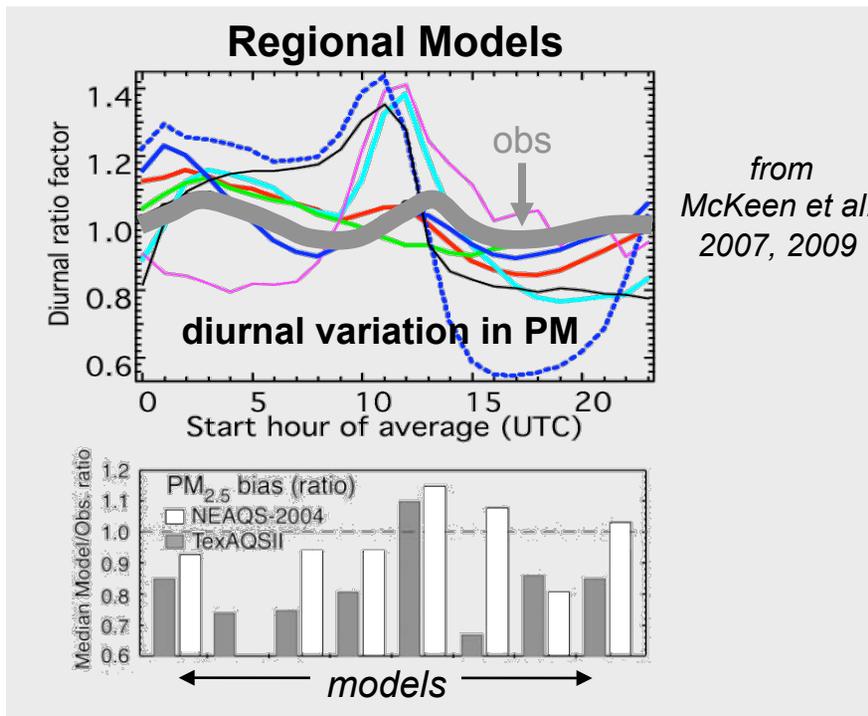
Many Models and Many Types of Evaluations



A More Systematic Approach is Needed

Current Aerosol Modeling Paradigm is Haphazard and Slow

- Differences among predictions arise from *many sources* (emissions, meteorology, chemistry, configuration) rather than aerosol treatments



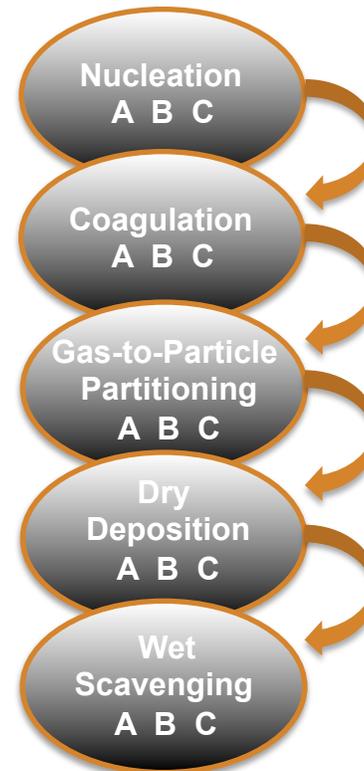
- Traditional model comparisons that quantify range of uncertainty often contain *little insight* on how to improve predictions
- Thus it is difficult *to improve* predictions in a timely manner

What Are We Trying to Accomplish?

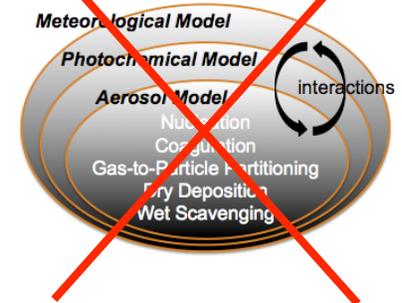
Create a computational framework, an **Aerosol Modeling Testbed**, that streamlines the process of testing and evaluating aerosol and clouds process modules over a range of spatial / temporal scales

- **Systematically and objectively** evaluate aerosol process modules
- Better **quantify uncertainties** by targeting specific processes
- Provide **tools** that facilitate science by minimizing redundant tasks
- **Document** performance and computational expense
- Build a capability that fosters **international collaboration**

New Modeling Paradigm



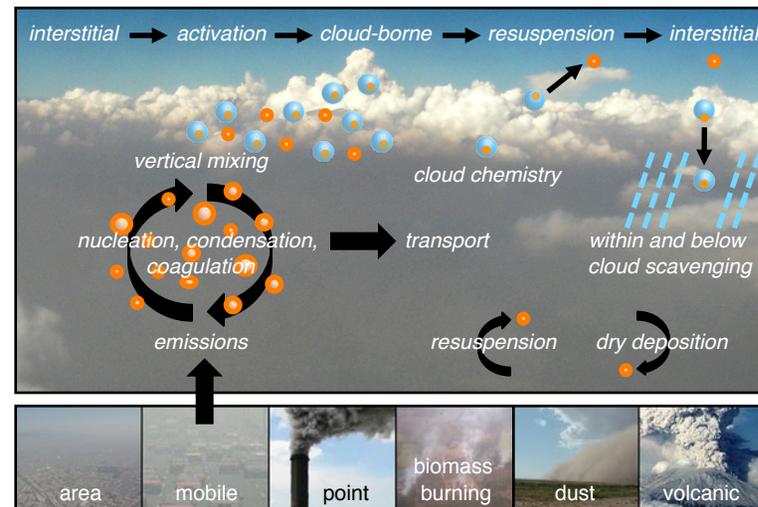
Traditional Modeling Paradigm



Approach

Use the **Weather Research and Forecasting (WRF)** model as the foundation of our computational framework

- Fully-coupled aerosol-radiation-cloud-chemistry interactions over multiple spatial scales
- Increasing international use
- Facilitates distribution of new process modules



Create a **community tool** in which aerosol process modules are evaluated systematically and objectively

- Target **specific** aerosol processes
- Assess performance by **fully** utilizing multiple field campaign datasets
- Long-term **archive** of model output
- Transparent code control, largely **automatic** but easily customized

Community Tools

Software that Enables Scientific Analysis

Extraction Programs – “Simulators”

extracts model variables compatible with a wide range of observation types

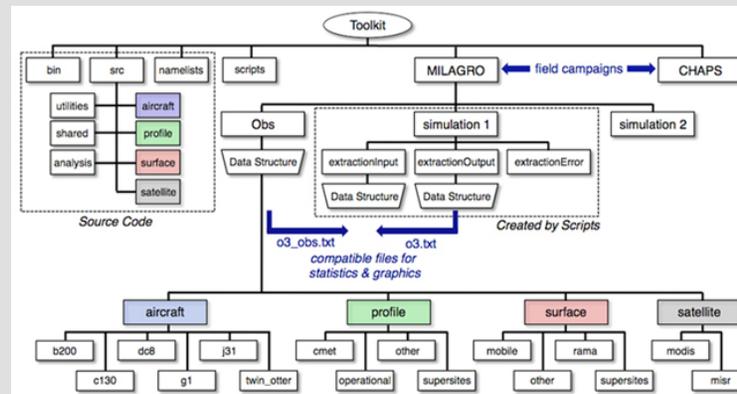


Analysis Programs

produces *graphics* and *statistics* that examines model performance

Parallel Structure - organizes data and model output

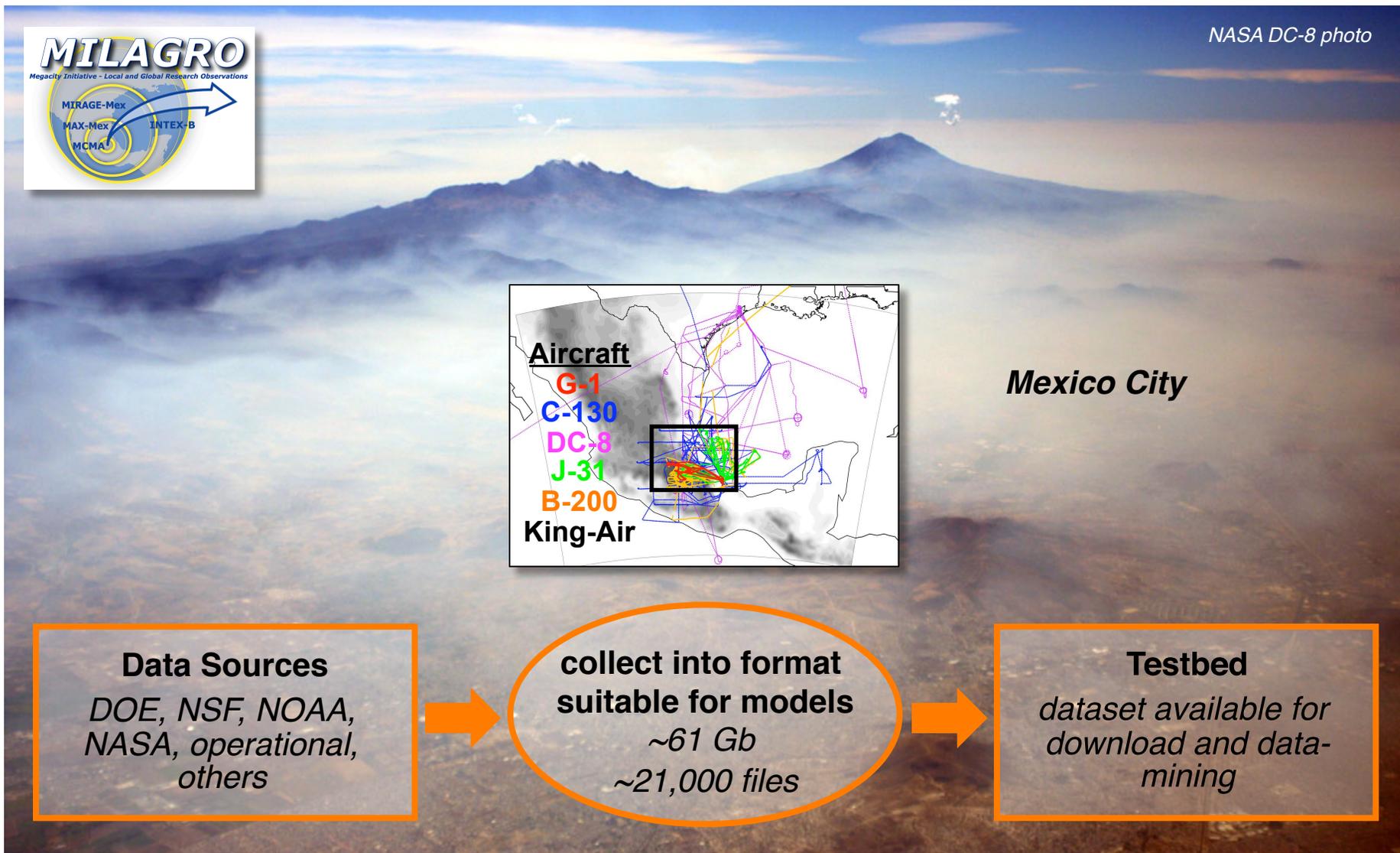
Scripts extract everything by default, but customizable



Minimize redundant tedious tasks normally performed by every modeler

First Testbed Case

Megacities Initiative: Local and Global Research Observations



Example: Simple versus Complex



Comparing Two Models in the Testbed

	MADE/SORGAM 	MOSAIC 
size distribution	modal (3 modes)	sectional (8 bins)
# of prognostic species	38 (76 with clouds)	104 (192 with clouds)

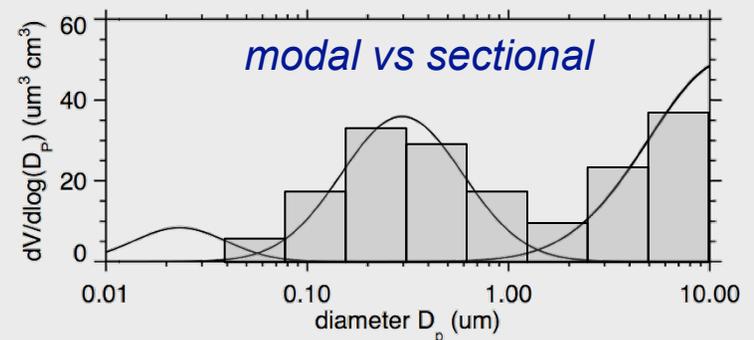
~ 2.7 

Identical:

- *Anthropogenic, biomass burning, online sea-salt & dust emissions*
- *Boundary conditions from global chemistry model (MOZART)*
- *Photochemistry (CBM-Z)*
- *SOA turned off*
- *Aerosol optical properties*
- *Aerosol-radiation-cloud interactions*
- *Dry deposition*

Differences:

- *Nucleation & coagulation*
- *Gas-to-particle partitioning: (equilibrium vs dynamic)*
- *Size distribution*

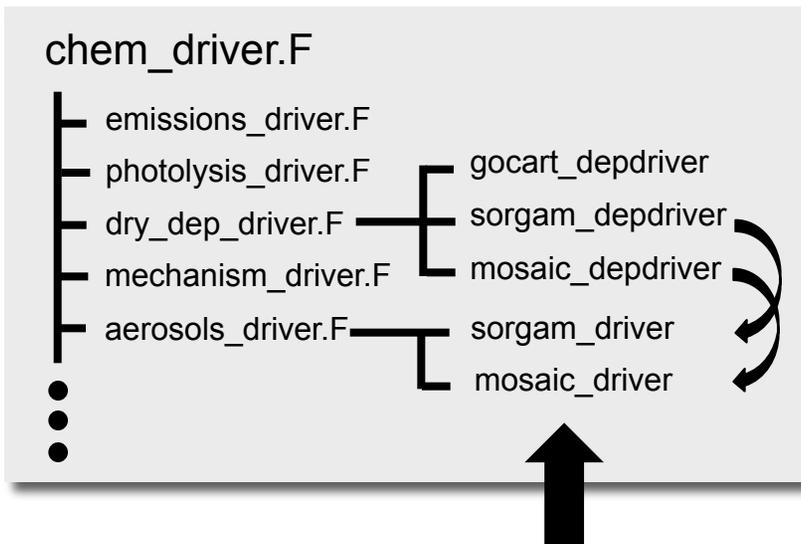


- *MOSAIC is ~1.83 times more computationally expensive*

Interoperability: Dry Deposition

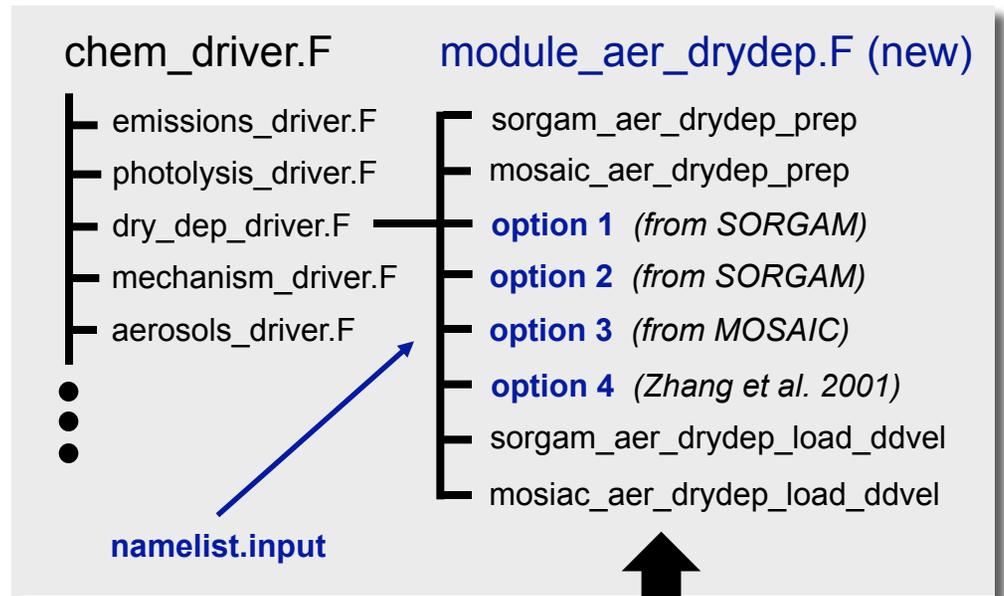
Flow Chart Demonstrating How Interoperability is Implemented

Flow Chart for WRF-Chem v3.1



each has different treatments;
code located in separate modules

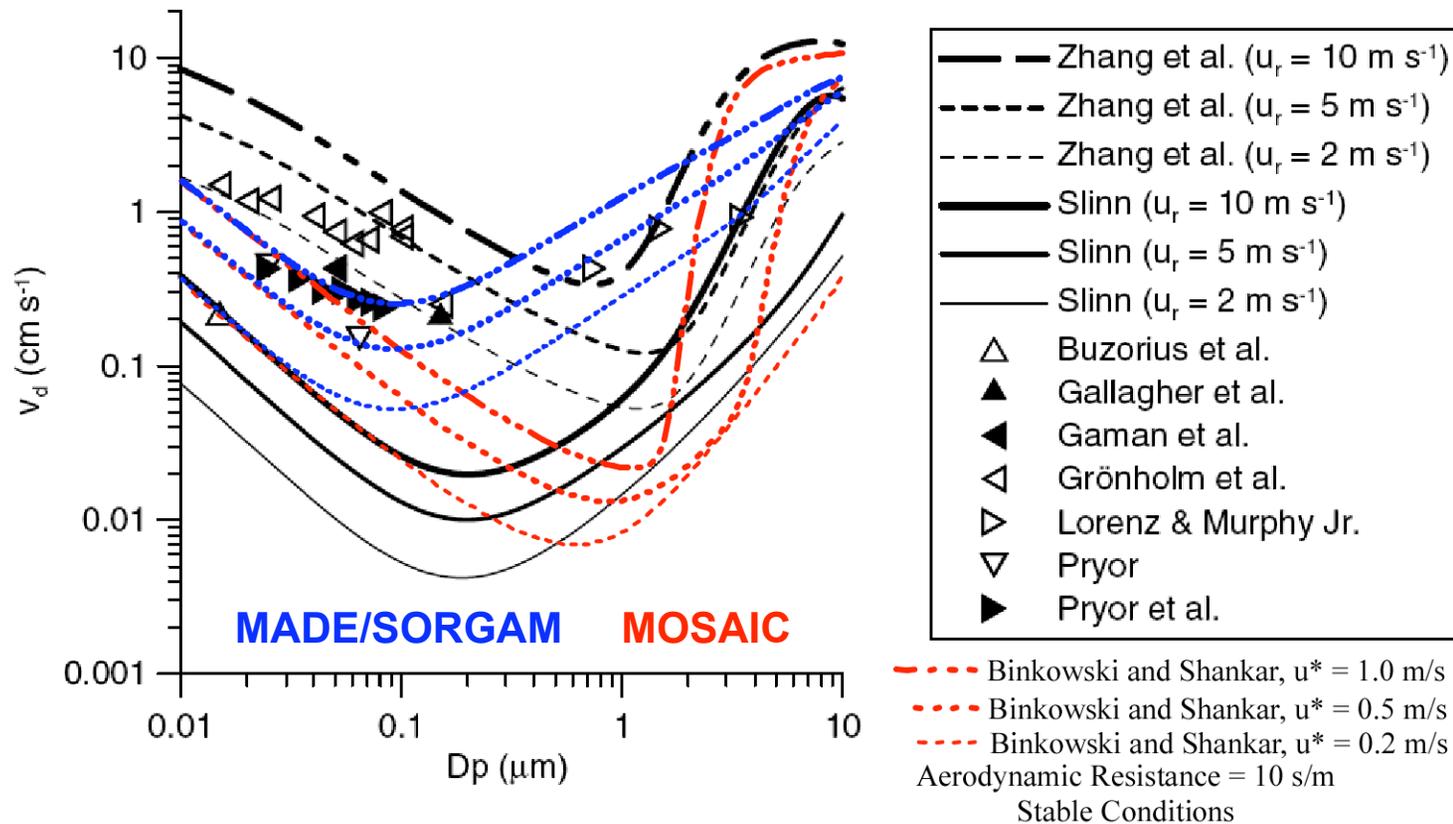
Flow Chart for AMT Branch



each option compatible with MADE/SORGAM
and MOSAIC; all code grouped into new
module, module_aer_drydep.F

Interoperability: Dry Deposition

Deposition Velocity for Evergreen Needleleaf Forest from Pryor et al., *Tellus*, 2008

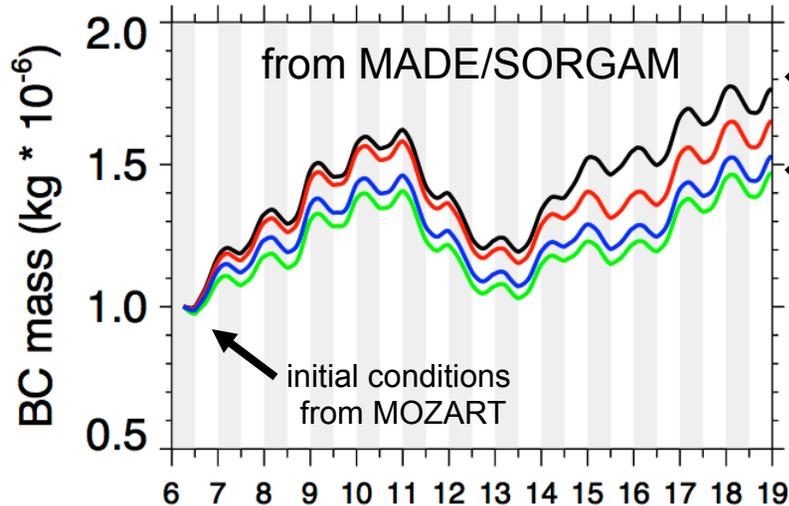


- v_d **varies greatly** among dry deposition treatments
- treatments based on **limited data** for specific vegetation types

Dry Deposition Uncertainties in Testbed Case

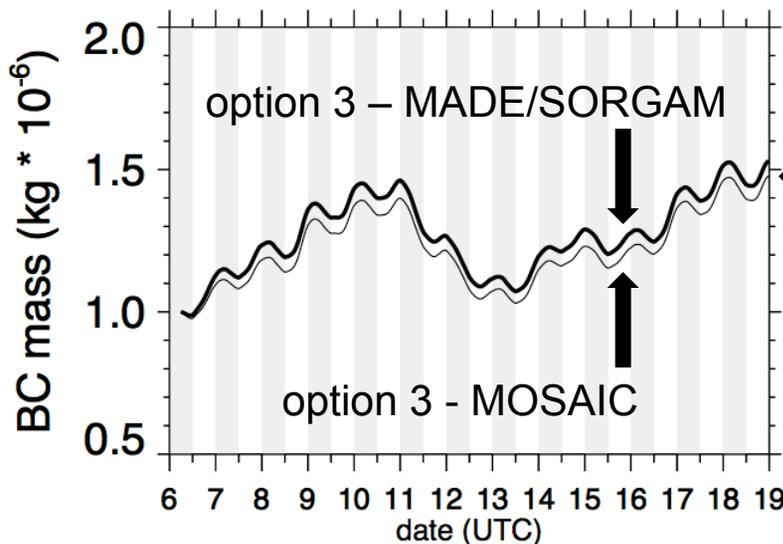
Black Carbon Mass

throughout entire model domain



models identical when deposition off
differences of ~12% among treatments

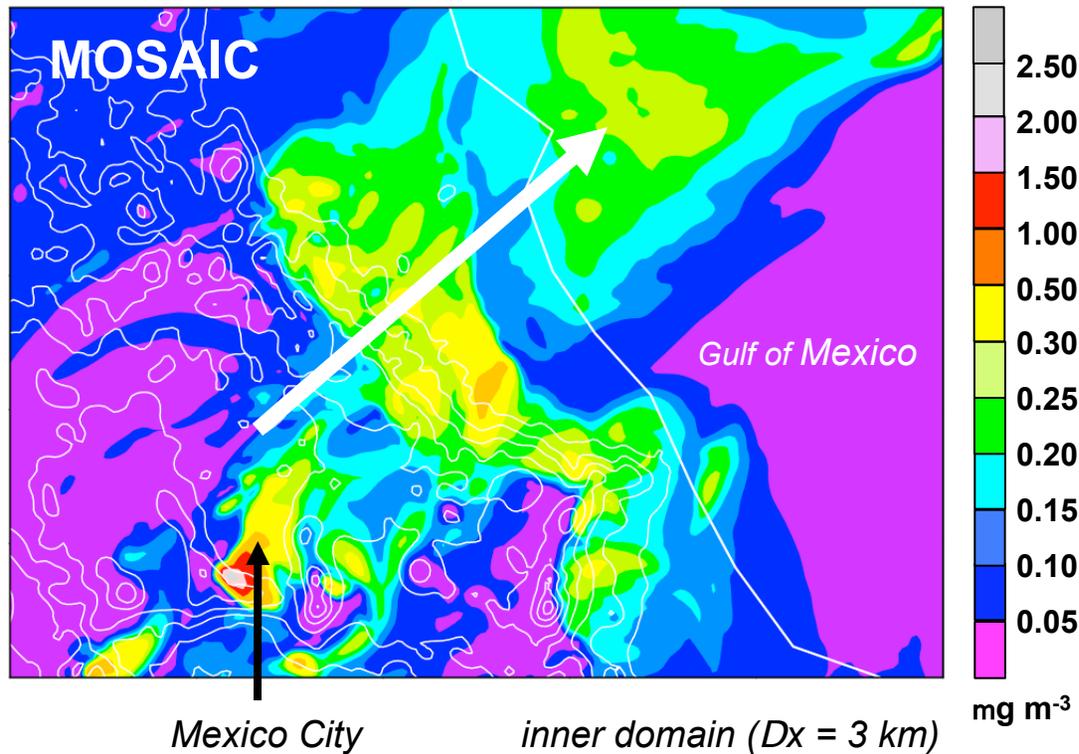
black = dry deposition off
option 1 (from MADE/SORGAM)
option 2 (from MOSAIC)
option 3 (from Zhang et al., 2001)] interoperable



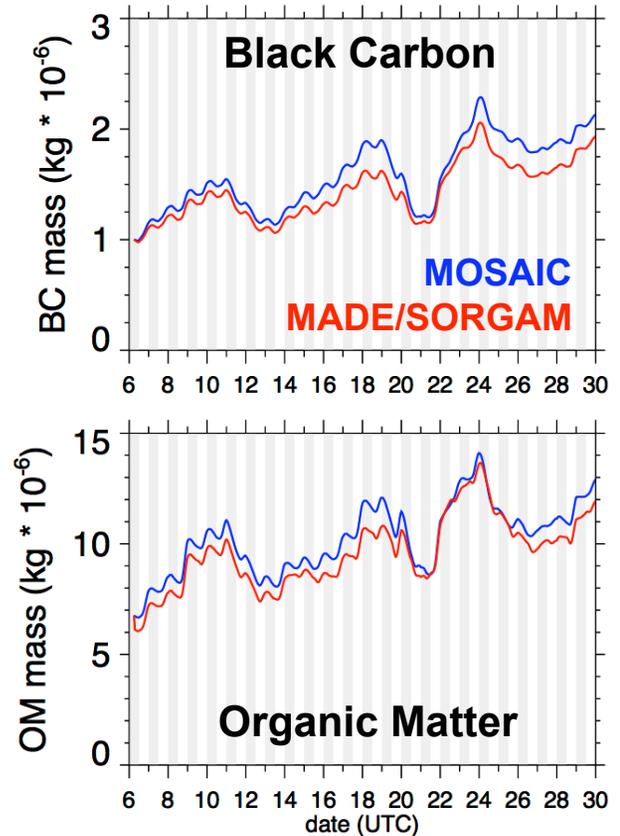
differences in size distribution produce differences of ~3%

Carbonaceous Aerosols

Black Carbon Concentrations ~1 km AGL 21 UTC March 20 – Strong Ambient SW Winds



Mass within Outer Domain dry deposition option 1

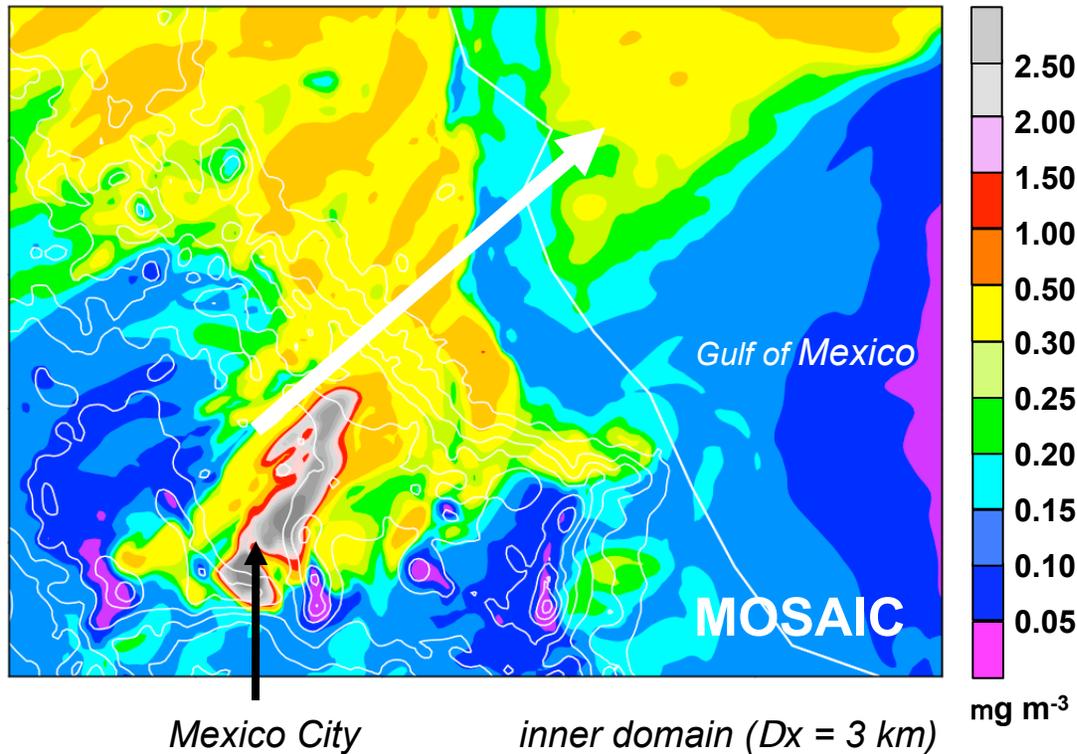


- Since BC and OM treated as a scalars with no chemistry (*SOA turned off*), differences due solely to **size distribution** in dry deposition and wet scavenging

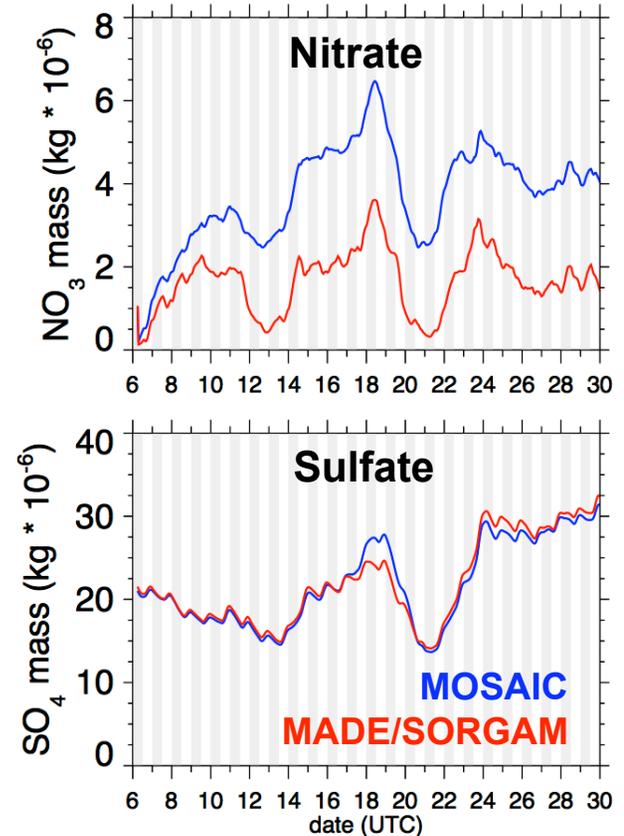
Secondary Aerosols

Nitrate Concentrations ~1 km AGL

21 UTC March 20 – Strong Ambient SW Winds



Mass within Outer Domain dry deposition option 1

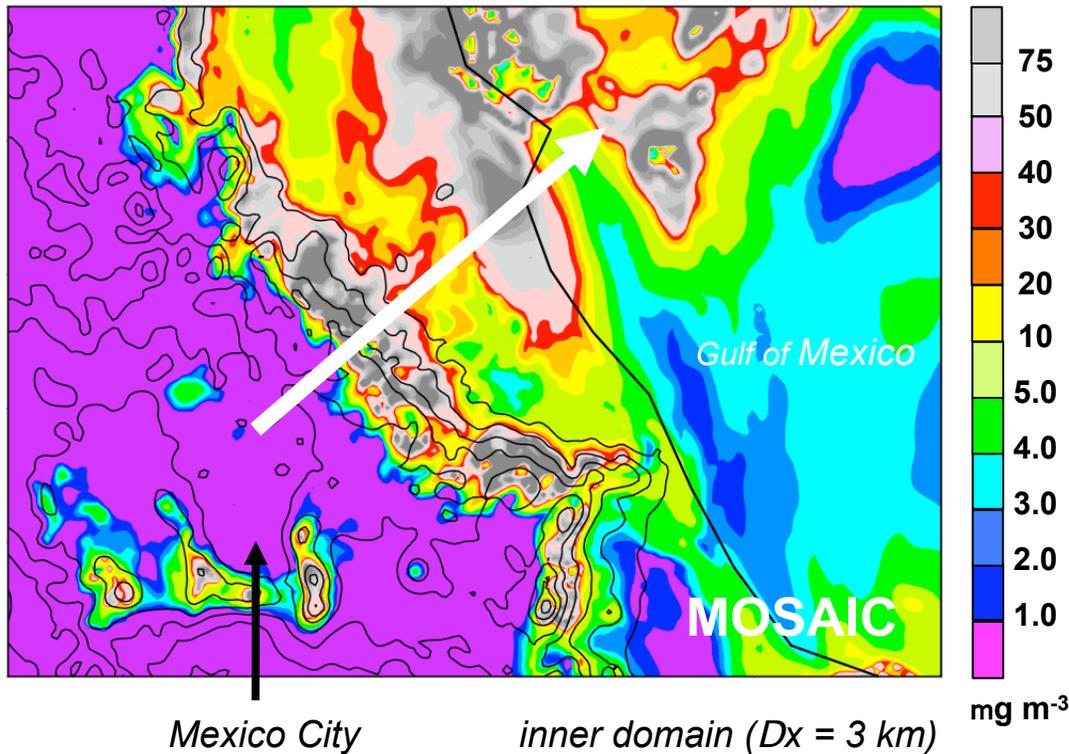


- Removal contributes, but different **gas-to-particle partitioning** treatments largely responsible
- $\text{HNO}_3 + \text{dust} \rightarrow$ coarse NO_3 included in MOSAIC

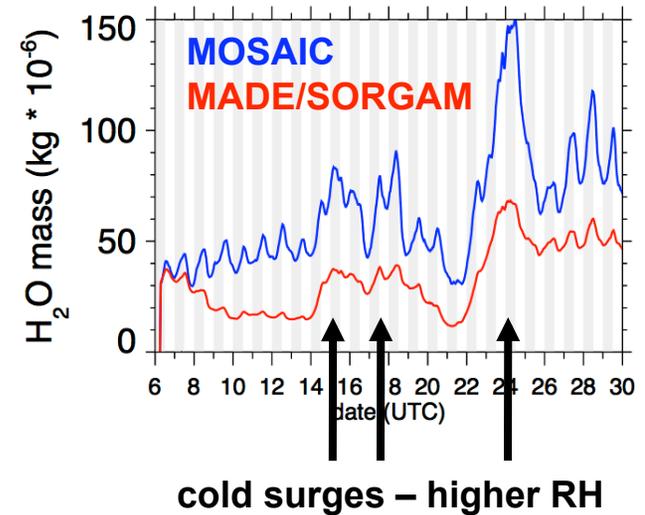
Aerosol Water

Aerosol Water ~1 km AGL

21 UTC March 20 – Strong Ambient SW Winds



H_2O within Outer Domain dry deposition option 1

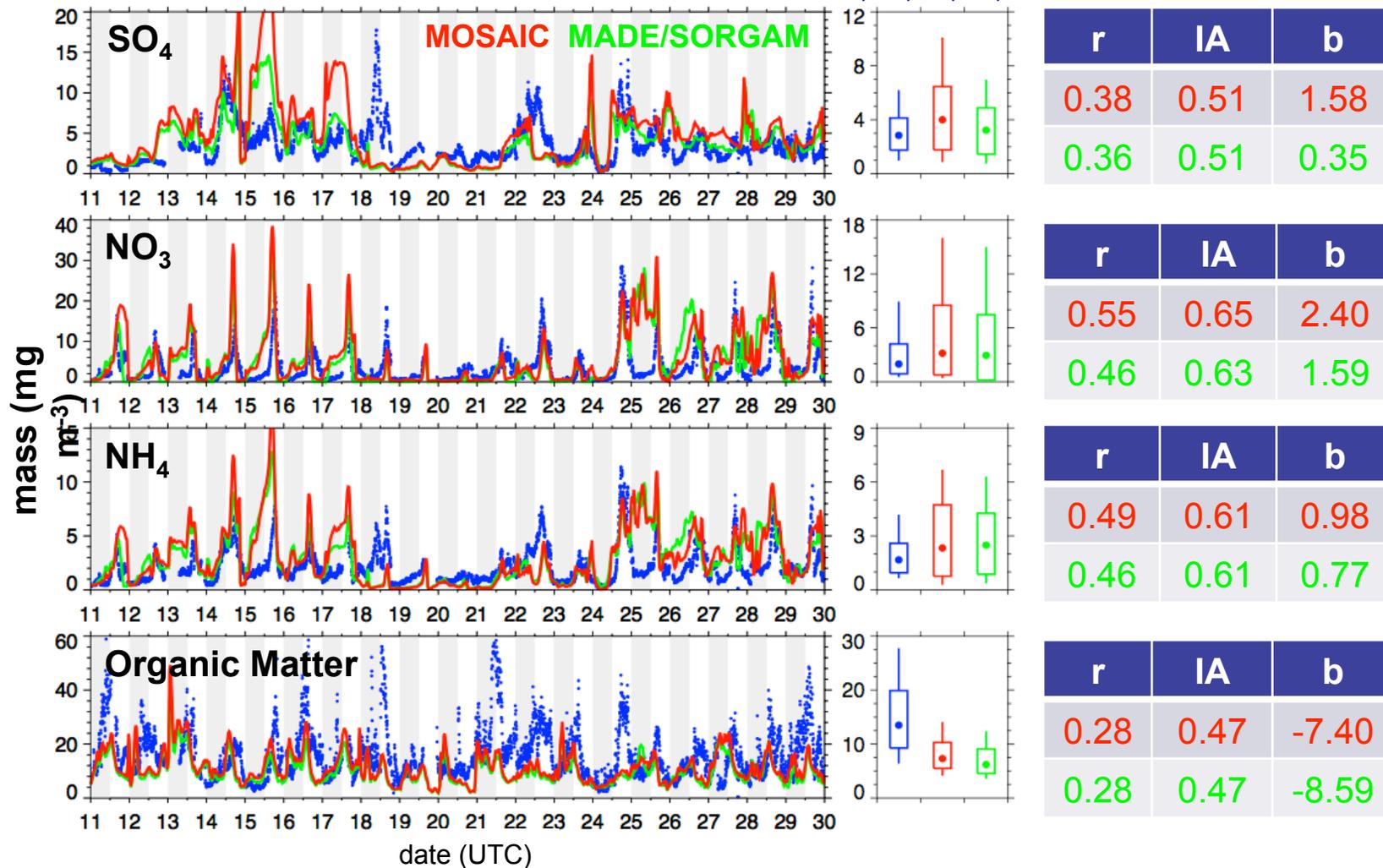


- Differences due to treatment of **gas-to-particle partitioning** and varying amounts of hydrophilic and hydrophobic aerosols

Aerosol Composition over Mexico City

AMS Observations at T0 Site

Percentiles
10, 25, 50, 75, 90

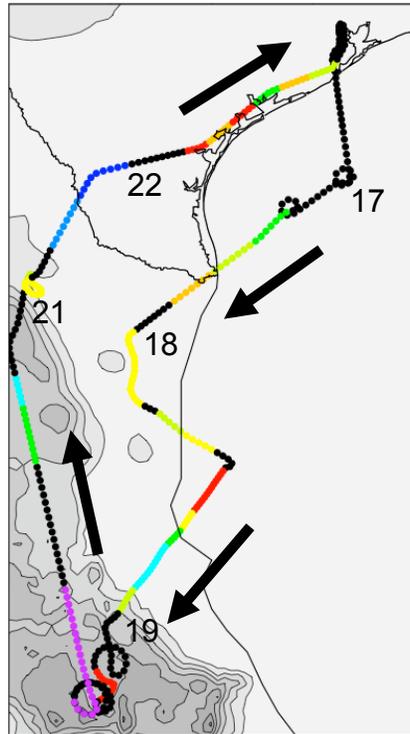


better agreement with HOA

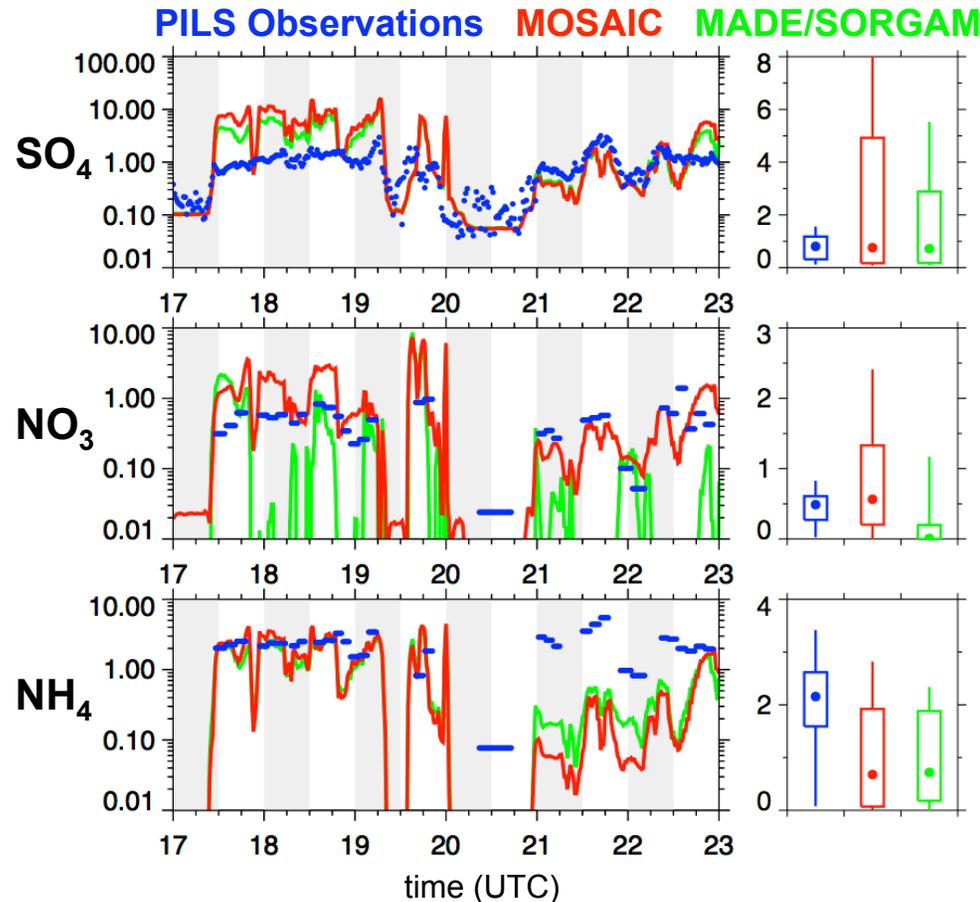
- Models **similar over the plateau**, close to the anthropogenic sources

Aerosol Composition Downwind of Mexico City

Along DC-8 Flight Path on March 19



red = highest NO_3 concentrations



r	IA	b
0.42	0.22	1.80
0.46	0.34	1.01

r	IA	b
0.46	0.37	0.46
0.22	0.38	-0.13

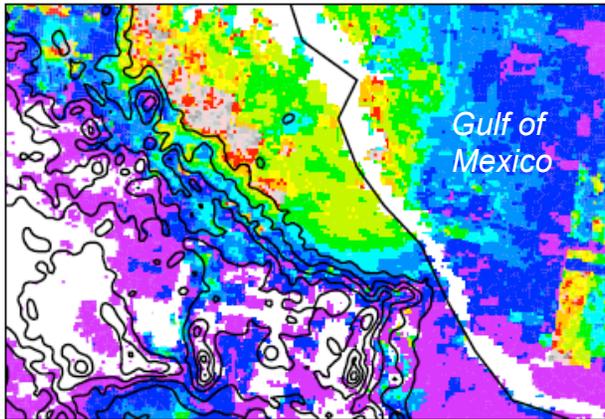
r	IA	b
0.14	0.49	-0.99
0.18	0.50	-1.10

- Meteorological errors contribute to plume displacements over Gulf ?
- MOSAIC somewhat better in predicting NO_3 downwind

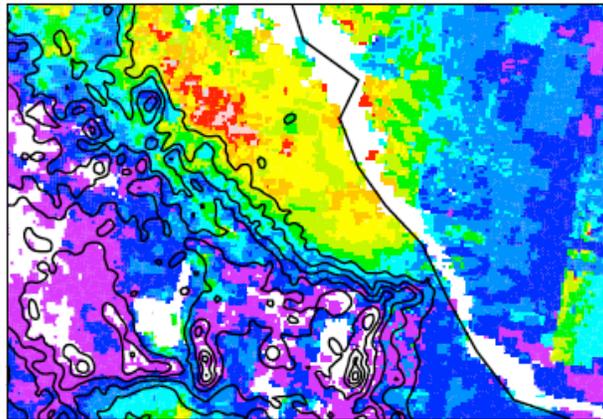
Satellite Simulator

Average AOD between March 6 and 29

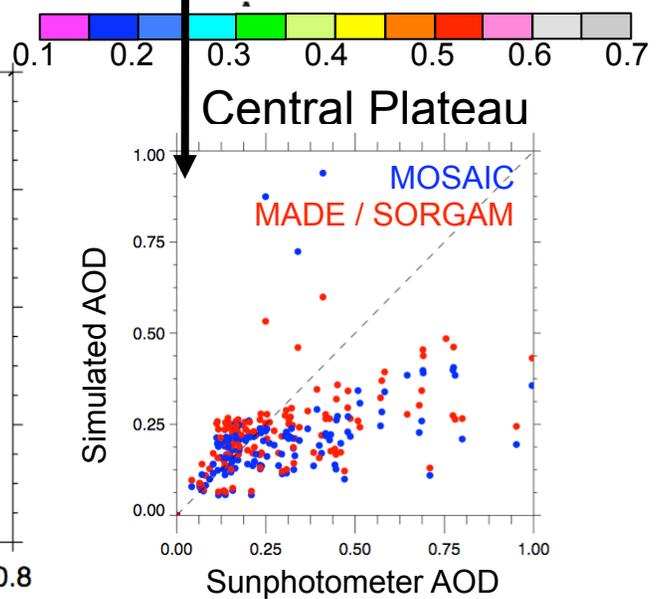
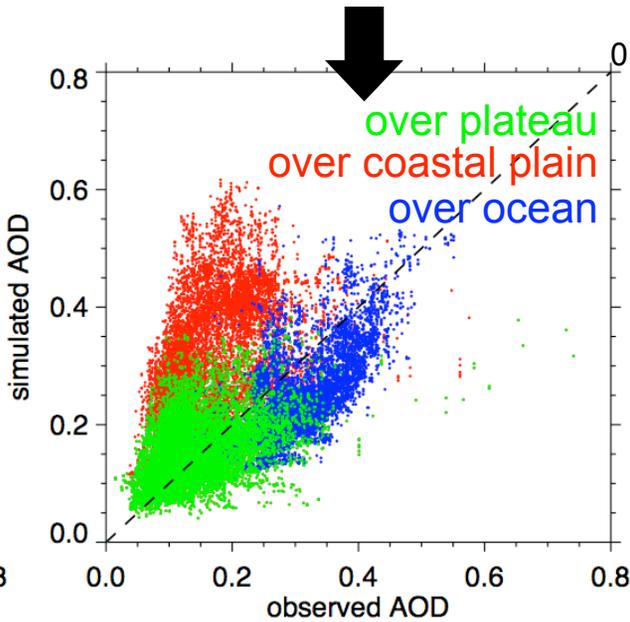
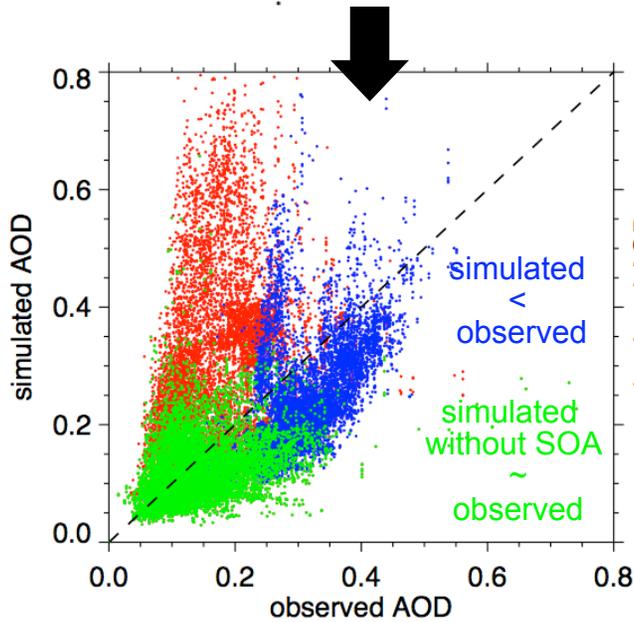
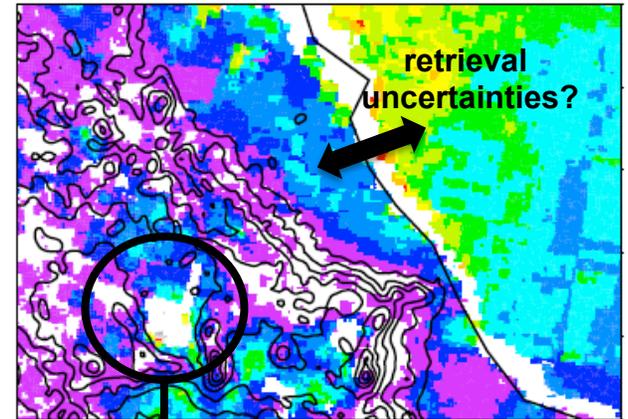
MOSAIC



MADE / SORGAM

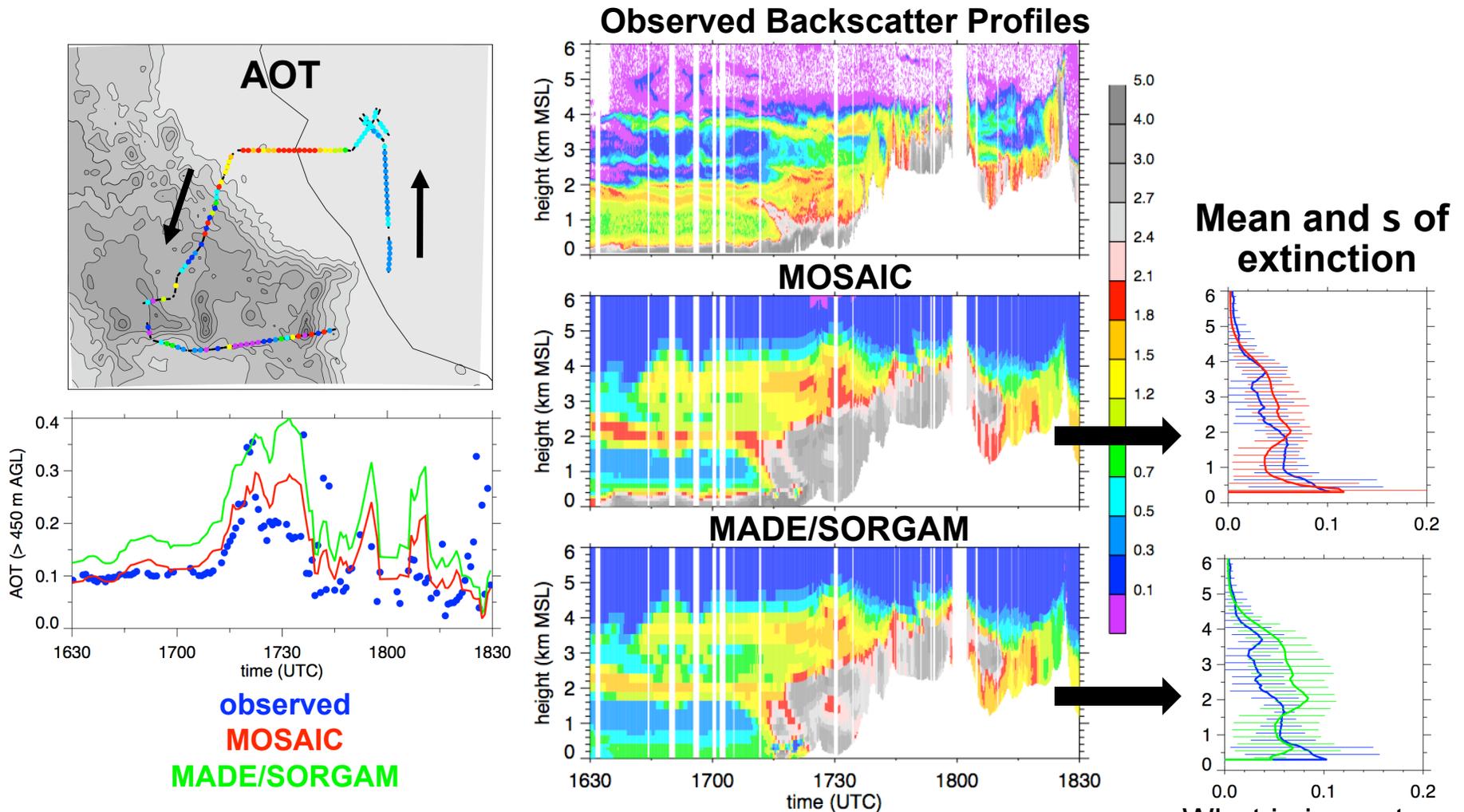


MODIS Terra



Lidar Simulator

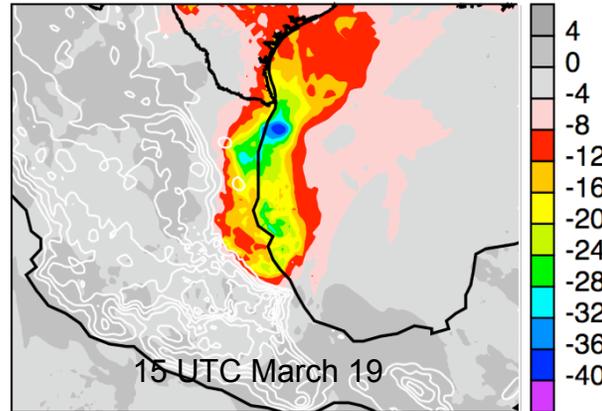
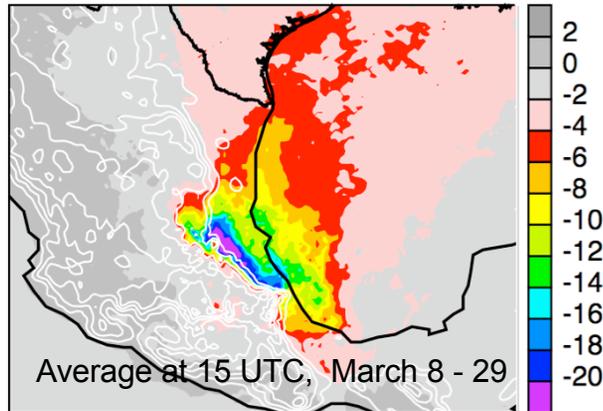
HRSL along the B-200 Flight Path on March 12



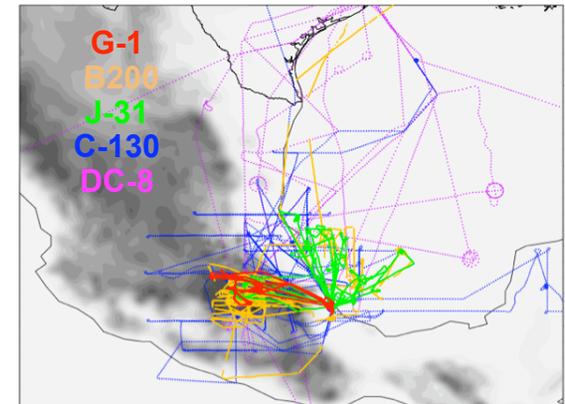
What is impact on heating rates?

Model Differences and Sampling

Difference in Net Shortwave Radiation (W m^{-2}) (MOSAIC – MADE/SORGAM)



All Aircraft Flight Paths



- Largest differences between the two models occurred where fewer aircraft measurements were obtained— useful to know these model differences *prior to* field campaign design and deployment
- Need to test *modal-MOSAIC* to isolate gas-to-particle partitioning
- Differences in SOA treatments will likely produce large differences close to Mexico City

What's Next?



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Testbed Cases Under Development

Multiple Cases Needed for Wide Range of Conditions



- **CHAPS / CLASIC:** processing of anthropogenic aerosols in shallow cumulus clouds

Oklahoma



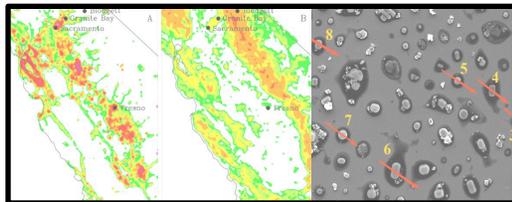
- **ISDAC:** processing of aged aerosols in Arctic mixed-phase clouds

**North Slope
of Alaska**



- **VOCALS:** processing of natural and anthropogenic aerosols in marine stratocumulus clouds

**southeastern
Pacific Ocean**



- **CARES / CALNEX:** secondary organic aerosols, black carbon mixing state, and their optical properties

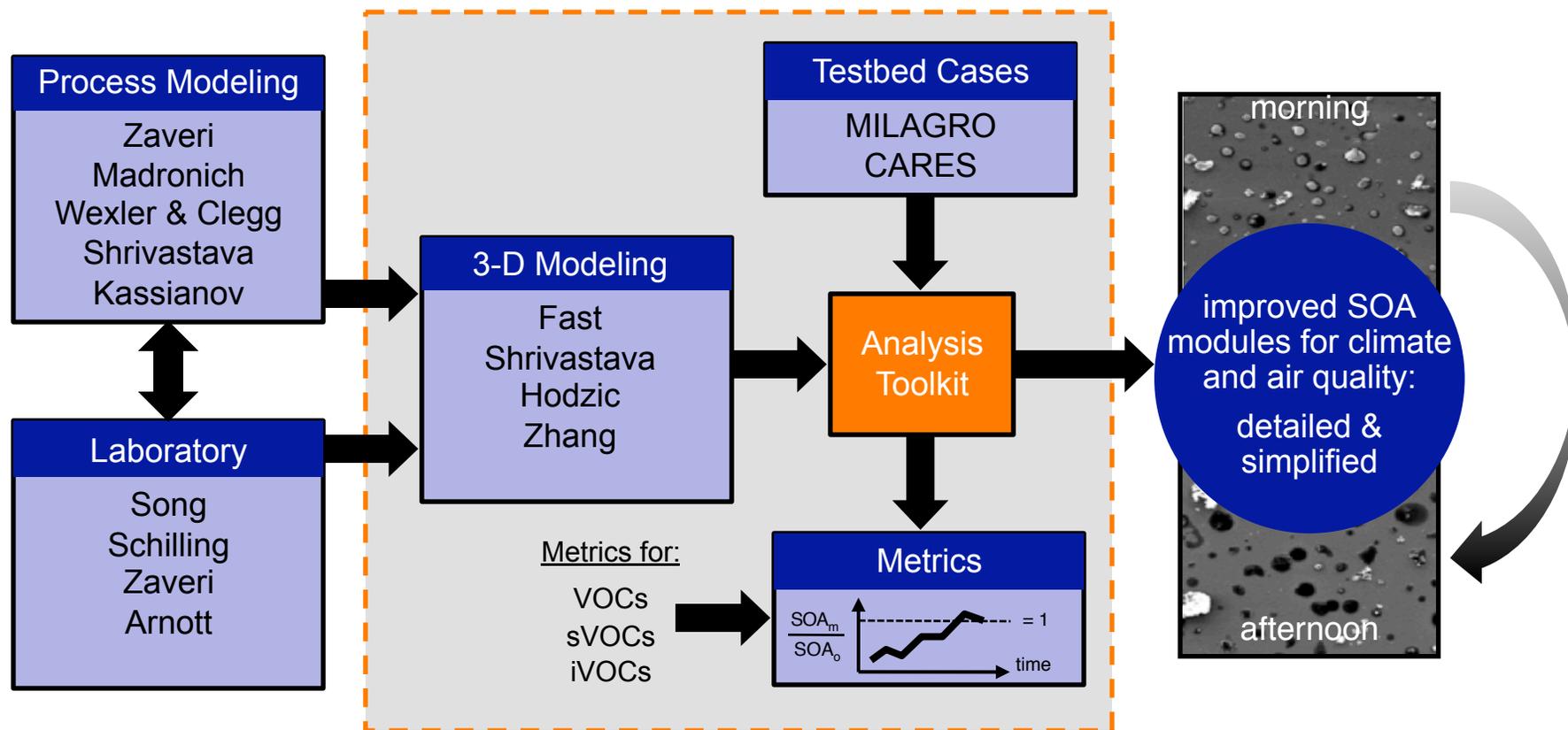
**California
(2010)**

- ICARTT, TexAQS, International Field Campaigns ?
- Users are free to develop their own cases for all to use

SOA Working Group

How will Field, Laboratory, and Modeling Scientists Work Together ?

Aerosol Modeling Testbed



- Working groups that target other specific processes could be established

Additional Information

Beta Testbed Web Site – Software and Testbed Case Now Available

<http://www.pnl.gov/atmospheric/research/aci/amt>

The screenshot shows the Pacific Northwest National Laboratory website. The main content area is titled "Aerosol Modeling Testbed" and features a section for "Analysis Toolkit: Example Graphics and Statistics for MILAGRO". Below this, there are two tables of data files, one for "Aircraft" and one for "Surface". Each table has a "Select Plot Type" dropdown menu and a "View" button for each file.

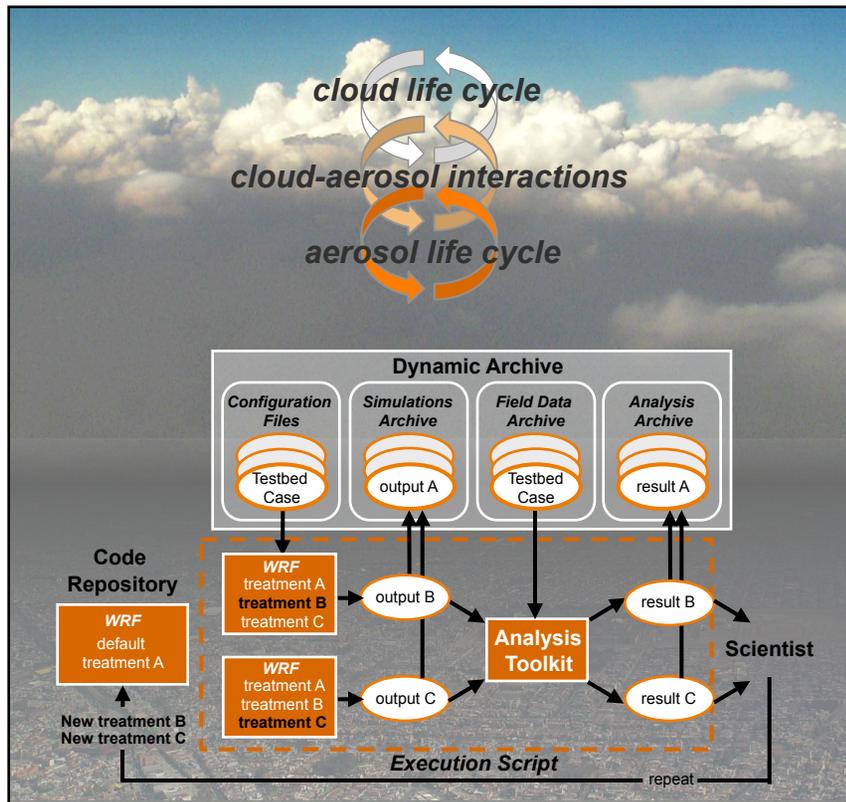
Aircraft	Select Plot Type: Time Series Scatter Percentile
Meteorology	<input type="text" value="timeser.potential_temperature.potential_temperature_obs.g1_060306"/> View »
Trace Gases	<input type="text" value="timeser.ald.ptrms_45_obs.g1_060306a.gif"/> View »
Hydrocarbons	<input type="text" value="timeser.ald.acetaldehyde_obs.mrg60_dc8_20060309_r5.gif"/> View »
Aerosols	<input type="text" value="timeser.Bin1_Aer_Number.dma_8binwrf_bin1number_obs.g1_060306a.gif"/> View »
Photolysis	<input type="text" value="timeser.PHOTR10.j_h2o2_2oh_obs.mrg60_c130_20060308_r4.gif"/> View »

Surface	Select Plot Type: Time Series Scatter Percentile
Meteorology	<input type="text" value="timeser.pressure.pressure_obs.mobile_ped_m4.gif"/> View »
Trace Gases	<input type="text" value="timeser.co.co_obs.mobile_ped_m4_qcl.gif"/> View »
Hydrocarbons	<input type="text" value="timeser.ald.acetaldehyde_obs.mobile_ped_m4_ptrms.gif"/> View »
Aerosols	<input type="text" value="timeser.aot340.aot340_obs.other_tamihua_aeronet.gif"/> View »
Photolysis	<input type="text" value="No Images Available"/> View »
Radiation	<input type="text" value="timeser.swdown.broadband_shortwave_downwelling_global_hemispheric"/> View »

- Basic overview
- Documentation describing how Analysis Toolkit software is run
- Example graphics and statistics
- How software and testbed cases can be downloaded

Article on the AMT to be submitted to BAMS in December

Summary



- AMT starting to be used for DOE climate research, and additional components are being developed
- Although the AMT's primary objective is to address climate models, ...
- It can also be used to improve aerosol process modules for air quality models

Acknowledgements:

- Support from PNNL Aerosol Climate Initiative and DOE Atmospheric Sciences Program
- Thanks to hundreds of scientists contributing to data used by testbed cases and development of WRF

Providing new modules with documented performance

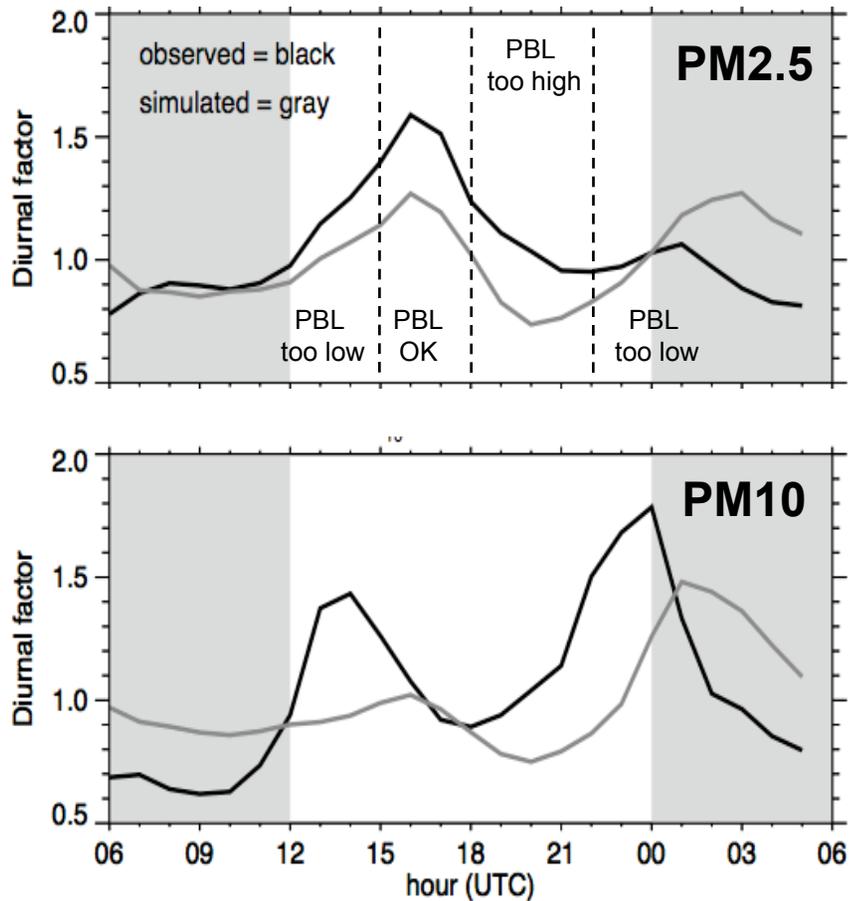
Testing modules at scales compatible with data

Global Climate Modeling Community

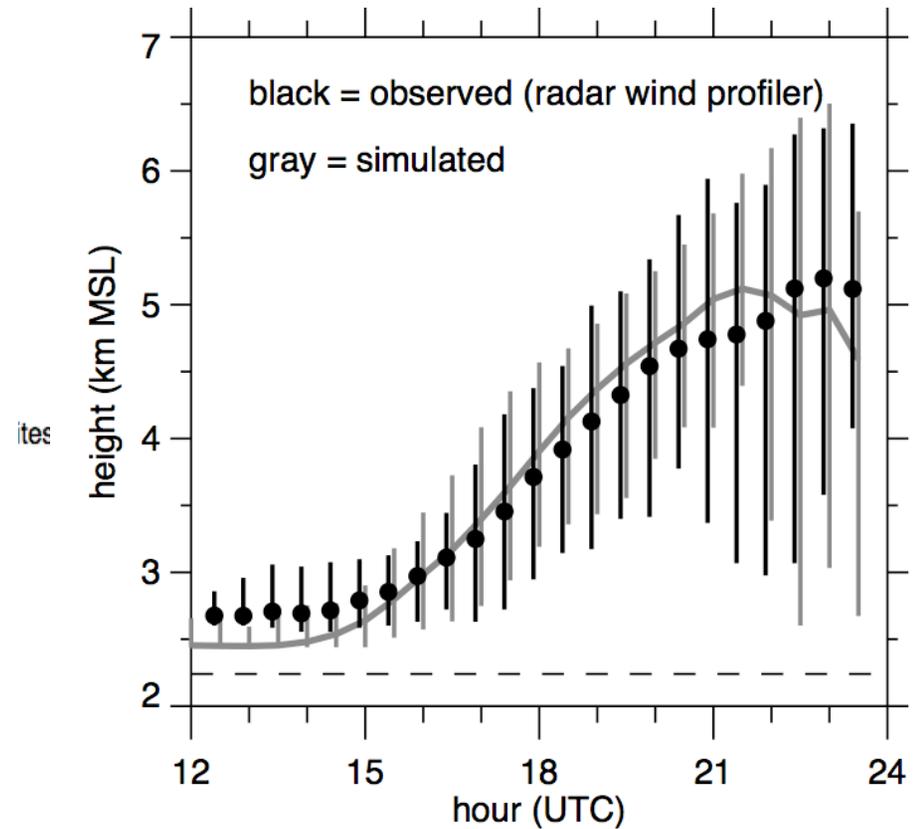
Extra Slides

PBL Depth and Dilution

Average Diurnal Variation in PM among RAMA monitoring sites

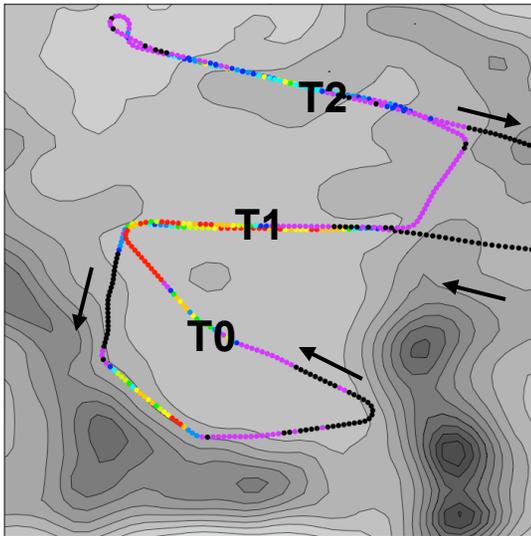


Average Variation in PBL Depth at T0 site



Aerosol Composition around Mexico City

NO₃ along G-1 Flight Path March 20



red = highest concentrations

AMS Observations MOSAIC MADE/SORGAM

